X FOURIER-TRANSFORMS AND ORTHONORMAL SYSTEMS

X.1 *Scalar products and orthogonality*

The fundamental idea of Fourier-transforms is the question whether a function can be represented as a linear combination of a parameterised family of base functions which acts as a basis system, very much like the representation of a vector in terms of its basis. For this purpose, one needs to generalise the notion of a projection to functions, i.e. one needs to define a sensible scalar product. Scalar products in vector spaces over $\mathbb{R}$ have the properties

1. positive definiteness:

   $\langle u, u\rangle \geq 0$, and $\langle u, u\rangle = 0$ implies $u = 0$

2. bilinearity:

   $\langle u, v_1 + v_2\rangle = \langle u, v_1\rangle + \langle u, v_2\rangle$ as well as $\langle u_1 + u_2, v\rangle = \langle u_1, v\rangle + \langle u_2, v\rangle$, and

   $\langle \alpha u, v\rangle = \alpha\langle u, v\rangle$ as well as $\langle u, \alpha v\rangle = \alpha\langle u, v\rangle$

3. symmetry:

   $\langle u, v\rangle = \langle v, u\rangle$

whereas in vector spaces over $\mathbb{C}$ there are slight differences,

1. positive definiteness:

   $\langle u, u\rangle \geq 0$, and $\langle u, u\rangle = 0$ implies $u = 0$

2. sesquilinearity (instead of bilinearity):

   $\langle u, v_1 + v_2\rangle = \langle u, v_1\rangle + \langle u, v_2\rangle$ as well as $\langle u_1 + u_2, v\rangle = \langle u_1, v\rangle + \langle u_2, v\rangle$, and

   $\langle u, \alpha v\rangle = \alpha\langle u, v\rangle$ but $\langle \alpha u, v\rangle = \alpha^*\langle u, v\rangle$ with a complex conjugation

3. hermiticity (instead of symmetry):

   $\langle u, v\rangle = \langle v, u\rangle^*$

In analogy to the scalar product in $\mathbb{R}^n$ one can define a scalar product for $\mathbb{R}$-valued functions in the interval $[a, b]$,

$$\langle u, v\rangle = u_i v^i \quad \rightarrow \quad \langle u, v\rangle = \int_a^b \mathrm{d}x\, u(x)v(x) \tag{X.495}$$

and for complex scalar products in $\mathbb{C}^n$ and $\mathbb{C}$-valued functions

$$\langle u, v\rangle = u_i^* v^i \quad \rightarrow \quad \langle u, v\rangle = \int_a^b \mathrm{d}x\, u^*(x)v(x) \tag{X.496}$$

with a complex conjugation.

The notion of orthogonality

$$\langle u^i, u_j\rangle \propto \delta^i_j \tag{X.497}$$

generalises straightforwardly to a set of functions $u^{(i)}(x)$ indexed by i, where we denote functions as vectors with a basis $|u_i\rangle$ and the associated linear forms with a basis $\langle u^i|$, borrowing the bra-ket notation from quantum mechanics.

If such as set should be able to approximate a function $g(x)$ in a linear combination

$$g(x) = a^i|u_i(x)\rangle \tag{X.498}$$

needs to make sure that the quadratic error Δ_N

$$\langle a_i u^i(x) - g(x)|a^j u_j(x) - g(x)\rangle \tag{X.499}$$

between the function and its approximation over the interval $[a,b]$ becomes small, and ideally vanishes in the limit $\mathrm{N}\to\infty$. It is sensible to integrate up the quadratic difference because the linear combination can over- or underestimate $g(x)$: Δ_N is positive definite and vanishes in the case of a perfect approximation.

$$\Delta_\mathrm{N} = a_i^* a^j\langle u^i, u_j\rangle - a_i^*\langle u^i, g\rangle - a^j\langle g, u_j\rangle + \langle g, g\rangle \tag{X.500}$$

If the basis system of functions $|u_i(x)\rangle$ is chosen to be orthogonal,

$$\langle u^i, u_j\rangle = \int_a^b \mathrm{d}x\, u^{(i)}(x)^* u^{(j)}(x) = \delta^i_j \tag{X.501}$$

the double sum in the first term collapses to a single sum, such that

$$\Delta_\mathrm{N} = a_i^* a^i - a_i^*\langle u^i, g\rangle - a^i\langle g, u_i\rangle + \langle g, g\rangle \tag{X.502}$$

The squared error Δ_N can be minimised with respect to a^k and a_k^*, which are mutually independent (think of them as being complex numbers, clearly the real and imaginary part are independent)

$$\frac{\partial}{\partial a^k}\Delta_\mathrm{N} = \underbrace{\frac{\partial a_i^*}{\partial a^k}}_{=0} a_i + a_i^*\underbrace{\frac{\partial a^i}{\partial a^k}}_{=\delta^i_k} - \underbrace{\frac{\partial a_i^*}{\partial a^k}}_{=0}\langle u^i, g\rangle - \underbrace{\frac{\partial a^i}{\partial a^k}}_{=\delta^i_k}\langle g, u_i\rangle + \underbrace{\frac{\partial}{\partial a^k}\langle g, g\rangle}_{=0} \tag{X.503}$$

such that

$$\frac{\partial}{\partial a_k}\Delta_\mathrm{N} = a_k^* - \langle g, u^k\rangle = 0 \quad\to\quad a_k{*} = \langle g, u^k\rangle = \int_a^b \mathrm{d}x\, g(x)^* u^{(k)}(x) \tag{X.504}$$

Similarly, minimisation with respect to a_k^* yields

$$\frac{\partial}{\partial a_k^*}\Delta_\mathrm{N} = \underbrace{\frac{\partial a_i^*}{\partial a_k^*}}_{=\delta_i^k} a^i + a_i^* \underbrace{\frac{\partial a^i}{\partial a_k^*}}_{=0} - \underbrace{\frac{\partial a_i^*}{\partial a_k^*}}_{=\delta_i^k} \langle u^i, g\rangle - \underbrace{\frac{\partial a_i}{\partial a_k^*}}_{=0} \langle g, u_i\rangle + \underbrace{\frac{\partial}{\partial a_k^*}\langle g, g\rangle}_{=0} \tag{X.505}$$

implying

$$\frac{\partial}{\partial a_k^*}\Delta_\mathrm{N} = a^k - \langle u_k, g\rangle \quad \rightarrow \quad a_k = \langle u_k, g\rangle = \int_a^b \mathrm{d}x\, u_k(x)^* g(x) \tag{X.506}$$

which is the hermitean conjugate of eqn. (X.504): When determining the expansion coefficients a_k of a complex function $g(x)$, one directly obtains *both* the real and imaginary part of a_k from the projection integral, so $a_k^* = \langle g, u_k\rangle$ and $a^k = \langle u^k, g\rangle$ are equivalent. In the case of a real-valued function $g(x)$, both a_k^* and a^k coincide, which implies that the coefficients themselves are real-valued.

With the coefficents a^i and a_i^* derived by projection, the value of the squared error Δ_N at the minimum is given by

$$\Delta_\mathrm{N}^{(\mathrm{min})} = \langle g, g\rangle - a_i^* a^i \tag{X.507}$$

which ideally would tend towards zero as $\mathrm{N} \rightarrow \infty$,

$$\lim_{\mathrm{N}\rightarrow\infty} \Delta_\mathrm{N}^{(\mathrm{min})} = \lim_{\mathrm{N}\rightarrow\infty} \langle a_i u^i - g, a^i u_i - g\rangle = 0 \quad \rightarrow \quad \langle g, g\rangle = \lim_{\mathrm{N}\rightarrow\infty} a_i^* a^i \tag{X.508}$$

referred to as convergence in the quadratic mean, implying the Parseval-relation, which is tightly related to the completeness relation of the basis system: After all, not all basis systems are able to make sure that the minimised mean quadratic error tends to zero.

$$a_i^* a^i = \langle g, u^i\rangle \langle u_i, g\rangle = \int_a^b \mathrm{d}x\, g(x)^* u_i(x) \int_a^b \mathrm{d}x'\, u^i(x')^* g(x') \tag{X.509}$$

Changing the integration order leads to

$$a_i^* a^i = \int_a^b \mathrm{d}x\, g(x)^* \int_a^b \mathrm{d}x'\, g(x')\, u^i(x')^* u_i(x) \tag{X.510}$$

If the system of functions fulfils

$$u^i(x)^* u_i(x') = \delta_D(x - x') \tag{X.511}$$

then one can continue to write

$$a_i^* a^i = \int_a^b dx\, g(x)^* \int_a^b dx'\, g(x')\delta_D(x - x') = \int_a^b dx\, g(x)^* g(x) = \langle g, g\rangle \tag{X.512}$$

and convergence is assured. This means, that the system of functions $|u^i(x)\rangle$ needs to be able to represent the Dirac δ_D-function. If that is the case, the system is complete for representing any function in the quadratic mean.

X.2 *Fourier-transforms*

Popular basis functions are plane waves because many differential equations in physics actually describe oscillations. In the finite interval $[-\pi, +\pi] \subset \mathbb{R}$, a discrete set of plane waves $u_n = \exp(\mathrm{i}nx)$ would be perfectly suited as a complete basis system, because

$$\sum_n^N \exp(\mathrm{i}nx)\exp(-\mathrm{i}nx') = \sum_n^N \exp(\mathrm{i}n(x - x')) =$$

$$\sum_n^N \exp(\mathrm{i}(x - x'))^n = \frac{\exp(\mathrm{i}(x - x')(N + 1)) - 1}{\exp(\mathrm{i}(x - x')) - 1} \tag{X.513}$$

as a consequence of the limit formula for geometric series, which can be reformulated to yield

$$= \exp\left(\mathrm{i}\frac{N}{2}(x - x')\right) \frac{\sin\left(\frac{N+1}{2}(x - x')\right)}{\sin\left(\frac{1}{2}(x - x')\right)} \sim \delta_D(x - x') \tag{X.514}$$

as the exponential becomes 1 in the limit $x \to x'$, the $\sin(x)/x$-function indeed approximates the Dirac δ_D-function. To show that the value at $x = x'$ is actually proportional to $N + 1$ requires the application of de l'Hôpital's rule for computing the limit $x \to x'$.

For the case of the infinite interval $(-\infty, +\infty)$ one can transition to a continuous set of basis functions. Introducing a wave vector $k = 2\pi/L$ for a plane wave $\exp(2\pi\mathrm{i}x/L) = \exp(\mathrm{i}kx)$ in the interval is likewise a complete basis system, and becomes continuous in the limit $L \to 0$. In fact,

$$\int_{-\pi/L}^{+\pi/L} \frac{dk}{2\pi} \exp(\mathrm{i}kx)\exp(\mathrm{i}kx')^* = \int_{-\pi/L}^{+\pi/L} \frac{dk}{2\pi} \exp(\mathrm{i}k(x - x')) = \frac{1}{2\pi}\frac{\exp(\mathrm{i}k(x - x'))}{\mathrm{i}(x - x')}\Bigg|_{-\pi/L}^{+\pi/L} \tag{X.515}$$

and evaluating the integral yields

$$= \frac{1}{\pi}\frac{\sin(\pi(x - x')/L)}{\pi(x - x')/L} \tag{X.516}$$

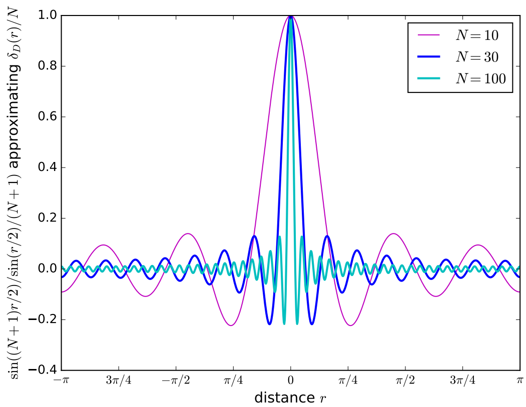

Figure 31: Eqn. X.516 as an approximation to the δ_D-function in the limit $\mathrm{N} \to \infty$.

which in the limit $\mathrm{L} \to 0$ behaves like the Dirac δ_D-function: The case of $x- \to x'$ can be sorted out by application of de l'Hôpital's rule, just as before in the discrete case.

In the continuum limit, the Fourier-transform $g(k)$ of a function $g(x)$ is given by

$$g(x) = \int \frac{\mathrm{d}k}{2\pi}\, g(k) \exp(+\mathrm{i}kx) \quad \leftrightarrow \quad g(k) = \int \mathrm{d}x\, g(x) \exp(-\mathrm{i}kx) \tag{X.517}$$

where you'll find in the literature any combination of distributing the factor 2π and choosing the sign in the wave $\exp(\pm \mathrm{i}kx)$. The two are really inverse, as

$$g(x) = \int \frac{\mathrm{d}k}{2\pi} \int \mathrm{d}x'\, g(x') \exp(\mathrm{i}k(x-x')) =$$
$$\int \mathrm{d}x'\, g(x') \int \frac{\mathrm{d}k}{2\pi} \exp(\mathrm{i}k(x-x')) = \int \mathrm{d}x'\, g(x')\delta_\mathrm{D}(x-x') = g(x) \tag{X.518}$$

illustrating the necessity of the 2π-factor. Generalising to more dimensions it becomes clear that the plane wave $\exp(\pm \mathrm{i}k_i r^i)$ factorises in Cartesian coordinates into $\exp(\pm \mathrm{i}k_x x)\exp(\pm \mathrm{i}k_y y)\exp(\pm \mathrm{i}k_z z)$, such that the Fourier-transform in n dimensions becomes a sequence of Fourier-transforms in 1 dimension:

$$g(\boldsymbol{r}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, g(\boldsymbol{k}) \exp(+\mathrm{i}k_i r^i) \quad \leftrightarrow \quad g(\boldsymbol{k}) = \int \mathrm{d}^3r\, g(\boldsymbol{r}) \exp(-\mathrm{i}k_i r^i) \tag{X.519}$$

Any further simplification is only possible if the function to be transformed itself factorises, too. The (scalar) product $\boldsymbol{k} \cdot \boldsymbol{r} = k_i r^i$ in index notation shows that k_i is in fact a linear form, which is foreshadowing quantum mechanics that sets $\hbar k_i = p_i$ with the momentum p_i.

X.3 *Convolutions with Fourier-transforms*

One of the primary applications of Fourier-transforms is to carry out convolutions $\varphi \otimes \psi$, as convolutions reduce to straightforward multiplications in Fourier-space.

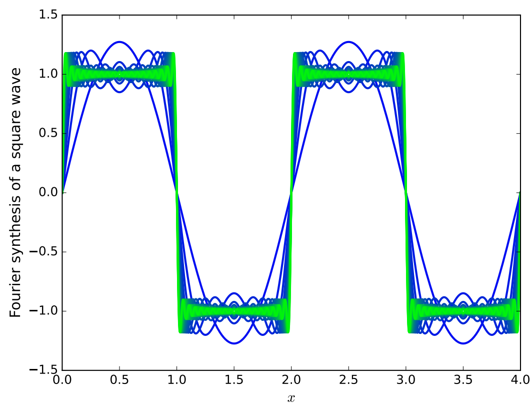

Figure 32: Square wave, assembled from the first 20 Fourier components.

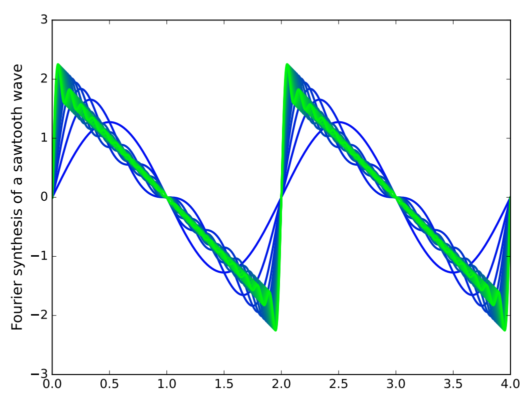

Figure 33: Sawtooth wave, assembled from the first 20 Fourier components.

Setting up a product $\varphi(\boldsymbol{k})\psi(\boldsymbol{k})$ between two Fourier-transformed functions $\varphi(\boldsymbol{k})$ and $\psi(\boldsymbol{k})$ and transforming back to configuration space yields

$$\varphi \otimes \psi(\boldsymbol{r}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, [\varphi(\boldsymbol{k})\psi(\boldsymbol{k})]\exp(+\mathrm{i}k_i r^i) \tag{X.520}$$

and substituting the forward-transformed fields gives

$$= \int \frac{\mathrm{d}^3k}{(2\pi)^3} \int \mathrm{d}V'\, \varphi(\boldsymbol{r}')\exp(-\mathrm{i}k_i r'^i) \int \mathrm{d}V''\, \psi(\boldsymbol{r}'')\exp(-\mathrm{i}k_j r''^j)\exp(+\mathrm{i}k_k r^k) \tag{X.521}$$

which, after reordering the integrations, is equivalent to

$$= \int \mathrm{d}V'\, \varphi(\boldsymbol{r}') \int \mathrm{d}V''\, \psi(\boldsymbol{r}'') \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, \exp(+\mathrm{i}k_i \cdot [\boldsymbol{r} - \boldsymbol{r}' - \boldsymbol{r}'']^i) \tag{X.522}$$

The d^3k-integration gives the Dirac δ_D-function, which fixes $\boldsymbol{r}''$ to the value $\boldsymbol{r} - \boldsymbol{r}'$,

$$= \int \mathrm{d}V'\, \varphi(\boldsymbol{r}') \int \mathrm{d}V''\psi(\boldsymbol{r}'')\delta_D(\boldsymbol{r} - \boldsymbol{r}' - \boldsymbol{r}'') = \int \mathrm{d}V'\, \varphi(\boldsymbol{r}')\psi(\boldsymbol{r} - \boldsymbol{r}') \tag{X.523}$$

i.e. a convolution, as advertised. Due to the perfect symmetry between Fourier-space and configuration space, the opposite is true as well: Convolutions in Fourier-space are products in configuration space.

X.4 *Green-functions with Fourier-transforms*

In the discussion of Poisson-type equations $\Delta\Phi = -4\pi\rho$ for solving potential problems we have seen that the potential Φ is given by a convolution of the charge distribution ρ with the Green-function G, which incidentally is $1/r$ for the Δ-operator in 3 dimensions:

$$\Phi(\boldsymbol{r}) = \int \mathrm{d}V'\, G(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}') = \int \mathrm{d}V'\, \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} \tag{X.524}$$

This convolution needs to become a product in Fourier-space

$$\Phi(\boldsymbol{k}) = G(\boldsymbol{k})\rho(\boldsymbol{k}) \quad \text{with} \quad G(\boldsymbol{k}) = \frac{4\pi}{k^2} \tag{X.525}$$

To obtain the expression for the Green-function G in configuration space it suffices to transform $G(k)$ back, where we make the replacement $\boldsymbol{r} - \boldsymbol{r}' \to \boldsymbol{r}'$, as the Green-function only depends on the relative distance:

$$G(\boldsymbol{r}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, G(k)\exp(+\mathrm{i}k_i r^i) \tag{X.526}$$

As $G(k) = 4\pi/k^2$ is spherically symmetric, it makes sense to carry out the integration in spherical coordinates: $\mathrm{d}^3k = k^2\mathrm{d}k\,\mathrm{d}\mu\,\mathrm{d}\varphi$ with $\mu = \cos\theta$ being the cosine of the polar angle θ:

$$G(\boldsymbol{r}) = \int_0^\infty \frac{k^2 \mathrm{d}k}{(2\pi)^3} \int_{-1}^{+1} \mathrm{d}\mu \int_0^{2\pi} \mathrm{d}\varphi \, \frac{4\pi}{k^2} \exp(+\mathrm{i}kr\mu) = \frac{4\pi}{(2\pi)^2} \int_0^\infty \mathrm{d}k \int_{-1}^{+1} \mathrm{d}\mu \, \exp(\mathrm{i}kr\mu) \quad \text{(X.527)}$$

because $k_i r^i = kr\cos\theta = kr\mu$, and because $\mathrm{d}\varphi$-integration just yields 2π. Next, the $\mathrm{d}\mu$-integration can be carried out to yield

$$= \frac{1}{\pi} \int_0^\infty \mathrm{d}k \, \frac{\exp(+\mathrm{i}kr) - \exp(-\mathrm{i}kr)}{\mathrm{i}kr} = \frac{2}{\pi} \int_0^\infty \mathrm{d}k \, \frac{\sin(kr)}{kr} = \frac{2}{\pi} \int_0^\infty \mathrm{d}k \, j_0(kr) = \frac{1}{r} \quad \text{(X.528)}$$

because the integral over $j_0(x) = \sin(x)/x$ can be shown to be

$$\int_0^\infty \mathrm{d}x \, \frac{\sin(x)}{x} = \frac{\pi}{2} \quad \text{(X.529)}$$

after substitution $x = kr$, usually with the methods of complex calculus (see chapter Y), but there are more down-to-Earth methods: There is **no** direct integration method for this type of integral, but neat tricks exist!

$$\int_0^\infty \mathrm{d}x \, \frac{\sin x}{x} = \int_0^\infty \mathrm{d}x \, \sin(x) \underbrace{\int_0^\infty \mathrm{d}y \, \exp(-yx)}_{=1/x} = \int_0^\infty \mathrm{d}y \int_0^\infty \mathrm{d}x \, \sin(x)\exp(-yx) \quad \text{(X.530)}$$

after changing the order of integration. The resulting $\mathrm{d}x$-integral can be solved by double integration by parts:

$$\int_0^\infty \mathrm{d}x \, \sin(x)\exp(-yx) = -\frac{1}{y}\sin(x)\exp(-yx)\Big|_0^\infty + \frac{1}{y}\int_0^\infty \mathrm{d}x \, \cos(x)\exp(-yx) \quad \text{(X.531)}$$

where the first term vanishes at both boundaries. Continuing with the second integration by parts yields

$$\ldots = -\frac{1}{y^2}\cos(x)\exp(-yx)\Big|_0^\infty - \frac{1}{y^2}\int \mathrm{d}x \, \sin(x)\exp(-yx) \quad \text{(X.532)}$$

where the first term in this case yields -1 at the lower integration boundary. Collecting the terms gives

$$\left(1 + \frac{1}{y^2}\right)\int_0^\infty \mathrm{d}x \, \sin(x)\exp(-yx) = \frac{1}{y^2} \quad \text{(X.533)}$$

such that

$$\int_0^\infty \mathrm{d}x \, \sin(x)\exp(-yx) = \frac{\frac{1}{y^2}}{1 + \frac{1}{y^2}} = \frac{1}{1 + y^2} \quad \text{(X.534)}$$

and finally

$$\int_0^\infty \mathrm{d}x\, \frac{\sin(x)}{x} = \int_0^\infty \mathrm{d}y\, \frac{1}{1+y^2} = \arctan(x)\Big|_0^\infty = \frac{\pi}{2} \tag{X.535}$$

The inverse problem and slight generalisation of the above calculation is the Fourier-transform of $1/r$,

$$\int_0^\infty r^2\mathrm{d}r \int_{-1}^{+1} \mathrm{d}\mu \int_0^{2\pi} \mathrm{d}\varphi\, \frac{1}{r}\exp(-\mathrm{i}kr\mu) \quad \rightarrow \quad \int_0^\infty r^2\mathrm{d}r \int_{-1}^{+1} \mathrm{d}\mu \int_0^{2\pi} \mathrm{d}\varphi\, \frac{\exp(-\lambda r)}{r}\exp(-\mathrm{i}kr\mu) \tag{X.536}$$

where the issue about convergence of the integral can be alleviated by introducing a factor $\exp(-\lambda r)$ to the integrand, and by considering the limit $\lambda \rightarrow 0$ after the integration: This method is known as regularisation of an integral. Physically, we compute the Fourier-transform of a Yukawa-potential instead of a Coulomb-potential. Continuing as before gives

$$\ldots = 4\pi \int_0^\infty r^2\mathrm{d}r\, \frac{\exp(-\lambda r)}{r}\frac{\sin(kr)}{kr} = \frac{4\pi}{k}\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\sin(kr) \tag{X.537}$$

The remaining integral can be solved again by double integration by parts: Firstly,

$$\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\sin(kr) = -\frac{1}{\lambda}\exp(-\lambda r)\sin(kr)\Big|_0^\infty + \frac{k}{\lambda}\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\cos(kr) \tag{X.538}$$

where the first term vanishes at both boundaries. Applying the second integration by parts on the remaining term yields

$$\frac{k}{\lambda}\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\cos(kr) = -\frac{k}{\lambda^2}\exp(-\lambda r)\cos(kr)\Big|_0^\infty - \frac{k^2}{\lambda^2}\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\sin(kr) \tag{X.539}$$

where at this step the first term vanishes at the upper, but not at the lower boundary. Consequently,

$$\left(1 + \frac{k^2}{\lambda^2}\right)\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\sin(kr) = \frac{k}{\lambda^2} \tag{X.540}$$

suggesting for the final result:

$$\frac{4\pi}{k}\int_0^\infty \mathrm{d}r\, \exp(-\lambda r)\sin(kr) = 4\pi\frac{\frac{1}{\lambda^2}}{1+\frac{k^2}{\lambda^2}} = \frac{4\pi}{k^2+\lambda^2} \rightarrow \frac{4\pi}{k^2} \quad \text{for} \quad \lambda \rightarrow 0 \tag{X.541}$$

Clearly, the inverse Fourier-transform of $4\pi/k^2$ should be $1/r$ (in three dimensions); as well in agreement with our experience with electrostatic potentials $\Phi \propto 1/r$ around point charges. The regularisation

$$\frac{1}{r} \rightarrow \frac{\exp(-\lambda r)}{r} \quad \text{corresponds to} \quad \frac{4\pi}{k^2} \rightarrow \frac{4\pi}{k^2+\lambda^2}, \tag{X.542}$$

and would work for inverse Fourier-transforms just as well.

A more professional method, which generalises to other types of Green-functions more easily, is to use the residue theorem from complex analysis. Restarting at

$$G(r) = \int_0^\infty \frac{k^2 \mathrm{d}k}{(2\pi)^3} \int_{-1}^{+1} \mathrm{d}\mu \int_0^{2\pi} \mathrm{d}\varphi \, \frac{4\pi}{k^2} \exp(+\mathrm{i}kr\mu) = \frac{2}{\pi} \int_0^\infty \mathrm{d}k \, \frac{\sin(kr)}{kr} \tag{X.543}$$

led us to the dk-integration over the spherical Bessel function. We can extend the integration domain from $-\infty$ to $+\infty$ as the integrand is a symmetric function, and write $\sin(x)$ out in terms of complex exponentials:

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, \frac{\sin x}{x} = \frac{1}{2\mathrm{i}} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{x} \, (\exp(\mathrm{i}x) - \exp(-\mathrm{i}x)) \rightarrow \frac{1}{2\mathrm{i}} \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{z} \, (\exp(\mathrm{i}z) - \exp(-\mathrm{i}z)) \tag{X.544}$$

by continuation to the complex plane. The two terms need to be treated differently when closing the integration to a loop: The first term $\exp(\mathrm{i}z)$ will decrease exponentially towards the positive imaginary axis, so one should close the integration contour there, while the second term $\exp(-\mathrm{i}z)$ decreases exponentially towards the negative imaginary axis, so this is where the loop should be closed. Keep in mind that the first loop is traversed in the mathematically positive sense, while the second one in the negative sense, leading in principle to negative results. Now, the integrand needs to get shifted by $\pm\mathrm{i}\epsilon$ with a small $\epsilon > 0$, such that the pole is contained in one of the integration contours and does not lie on the real axis. Let's chose to move the integrand towards the positive imaginary axis by changing z to $z - \mathrm{i}\epsilon$. In this case, only the first term contributes to the integral (with the integration contour $\frown$) as the second integration contour ($\smile$) does not contain the pole and is therefore zero:

$$\frac{1}{2\mathrm{i}} \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{z} \, (\exp(\mathrm{i}z) - \exp(-\mathrm{i}z)) = \frac{1}{2\mathrm{i}} \oint_{\frown} \frac{\mathrm{d}z}{z} \exp(\mathrm{i}z) + \frac{1}{2\mathrm{i}} \oint_{\smile} \frac{\mathrm{d}z}{z} \exp(-\mathrm{i}z) \tag{X.545}$$

Simplifying the relation further, the loop-integral can be solved with Cauchy's integral formula:

$$\oint_\Gamma \mathrm{d}\zeta \, \frac{g(\zeta)}{\zeta - z} = 2\pi\mathrm{i} \, g(z) \tag{X.546}$$

with ζ set to zero. As $\exp(\mathrm{i}\zeta) = 1$ at this location, the sought integral bocomes

$$2 \int_0^\infty \mathrm{d}x \, \frac{\sin x}{x} = \int_{-\infty}^{+\infty} \mathrm{d}x \, \frac{\sin x}{x} = \frac{1}{2\mathrm{i}} \oint_{\frown} \frac{\mathrm{d}z}{z} \exp(\mathrm{i}z) = \pi. \tag{X.547}$$

Fig. 34 illustrates the integrand of the Green-function for Δ in Fourier-space, with the singularity at the origin.

While these methods generalise straightforwardly to $n \geq 4$, the case of $n = 2$ is downright weird. The corresponding Poisson-equation reads

$$\Delta\Phi = -2\pi\rho \quad \text{in } \textit{two} \text{ dimensions,} \tag{X.548}$$

because the solid angle element in 2d is 2π, as the circumference of a circle with unit radius. But the Fourier-transform of Δ is still $\propto 1/k^2$ as shown before, only that $k^2 = k_x^2 + k_y^2$ in 2 dimensions. Writing formally

$$G(\boldsymbol{r}) = 2\pi \int \frac{d^2k}{(2\pi)^2}\frac{1}{k^2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) = \int_0^\infty k\,dk \int_0^{2\pi} d\varphi\,\frac{1}{k^2}\exp(ikr\cos\varphi) \tag{X.549}$$

after introducing polar coordinates that imply $d^2k = k\,dk\,d\varphi$, and writing the scalar product as $\boldsymbol{k}\cdot\boldsymbol{r} = kr\cos\varphi$, with φ being the angle between $\boldsymbol{k}$ and $\boldsymbol{r}$. Carrying out the $d\varphi$-integration first leads to the cylindrical Bessel-function J_0, because

$$J_0(kr) = \int_0^{2\pi} d\varphi\,\exp(ikr\cos\varphi) \tag{X.550}$$

such that

$$G(\boldsymbol{r}) = \int_0^\infty \frac{dk}{k} J_0(kr) \rightarrow \int_0^\infty dk\,\frac{k}{k^2+\lambda^2} J_0(kr) \tag{X.551}$$

by introducing a regularisation in the denominator, which avoids the divergence at $k = 0$. Integrations of this type have the general solution

$$\int_0^\infty dk\,\frac{k^{\nu+1}}{(k^2+\lambda^2)^{\mu+1}} J_\nu(kr) = \frac{r^\mu\lambda^{\nu-\mu}}{2^\mu\Gamma(\mu+1)} K_{\nu-\mu}(\lambda r) = K_0(r\lambda) \quad \text{with } \nu = \mu = 0 \tag{X.552}$$

in our particular case, with $K_0(r\lambda)$ being the modified Bessel-function of the second kind,

$$K_0(r\lambda) = \int_0^\infty dt\,\frac{\cos(r\lambda t)}{\sqrt{1+t^2}}. \tag{X.553}$$

This particular Bessel-function can be written in terms of a power series in its argument $r\lambda$. In the limit of vanishing regularisation, the value of the power series is dominated by its first term:

$$K_0(r\lambda) = -\left(\ln(r\lambda) + \gamma\right) I_0(r\lambda) \tag{X.554}$$

with $I_0(r\lambda)$ as the modified Bessel function of the first kind approaching unity in the limit $\lambda \rightarrow 0$, leaving $G(r) \propto \ln(r)$. γ is ✈ Euler's constant.

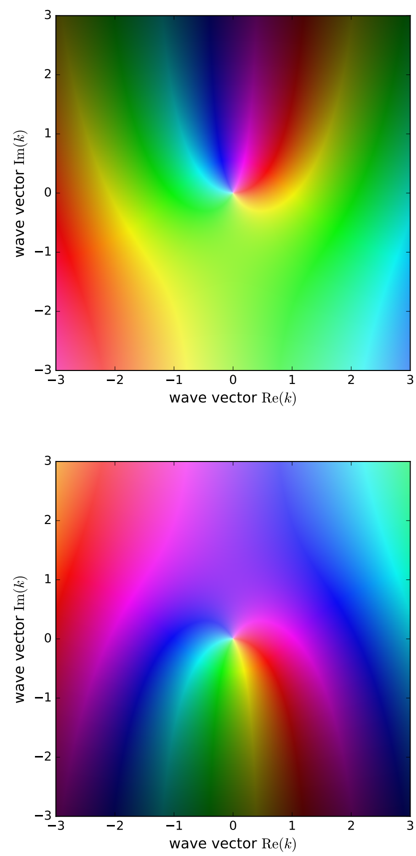

Figure 34: Function $\exp(\pm \mathrm{i}k)/k$ *over the complex plane* $k = \mathrm{Re}(k) + \mathrm{i}\,\mathrm{Im}(k)$*, with color indicating phase and hue indicating the absolute value, for the positive sign the exponent (decreasing towards the positive imaginary axis) on the top and the negative sign (decreasing towards the negative imaginary axis) on the bottom. The singularity at the origin is clearly visible.*

X.5 *Spectra of musical instruments*

An externally driven oscillator illustrates nicely the purpose of a Green-function to cope with inhomogeneities: Let's work with a harmonic oscillator with proper frequency ω_0, a damping γ driven by an external acceleration $a(t)$. Its defining differential equation is

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x(t) = a(t) \tag{X.555}$$

Finding a solution for the homogeneous equation is straightforward: The ansatz $x(t) \propto \exp(\mathrm{i}\omega t)$ yields the characteristic equation $\omega^2 - \mathrm{i}\omega\gamma - \omega_0^2 = 0$, with two solutions, $\omega_\pm = \left(\mathrm{i}\gamma \pm \sqrt{\gamma^2 - 4\omega_0^2}\right)/2$. Effectively, this corresponds to taking the Fourier-transform of the differential equation, which then becomes algebraic:

$$\int \frac{\mathrm{d}\omega}{2\pi} \left[-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2\right] \exp(\mathrm{i}\omega t) x(\omega) = 0 \tag{X.556}$$

as the differentiation $\mathrm{d}/\mathrm{d}t$ replaces the prefactor $\mathrm{i}\omega$, such that we recover the quadratic characteristic equation again. The incorporation of the inhomogeneity can easily be achieved in Fourier-space:

$$\int \frac{\mathrm{d}\omega}{2\pi} \left[-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2\right] \exp(\mathrm{i}\omega t) x(\omega) = \int \frac{\mathrm{d}\omega}{2\pi} a(\omega) \exp(\mathrm{i}\omega t). \tag{X.557}$$

Because the differential equation has become algebraic, solving for $x(\omega)$ is easy:

$$x(\omega) = \frac{1}{-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2} a(\omega) = \mathrm{G}(\omega) a(\omega) \tag{X.558}$$

such that the inverse Fourier-transform yields $x(t)$ for a given driving term $a(t)$. The product relation in Fourier-space must be a convolution in real space,

$$x(t) = \int \frac{\mathrm{d}\omega}{2\pi} \frac{1}{-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2} a(\omega) \exp(\mathrm{i}\omega t) = \int \mathrm{d}t'\, \mathrm{G}(t - t') a(t') \tag{X.559}$$

where the inverse differential operator is just the Green-function for this problem:

$$\mathrm{G}(t - t') = \int \frac{\mathrm{d}\omega}{2\pi} \frac{1}{-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2} \exp(\mathrm{i}\omega(t - t')) \tag{X.560}$$

$\mathrm{G}(\omega)$ or equivalently, $\mathrm{G}(t - t')$ determines the response of the system, i.e. the damped harmonic oscillator, to an external driving. Most obviously, this is understood in Fourier-space, where $\mathrm{G}(\omega)$ translates the driving $a(\omega)$ to the resulting amplitude $x(\omega)$, frequency by frequency. In configuration space, $\mathrm{G}(t - t')$ is likewise the response of the system, and it is defined formally as the solution to the differential equation to a δ_D-like inhomogeneity,

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\right) \mathrm{G}(t - t') = \delta_\mathrm{D}(t - t') \tag{X.561}$$

because any inhomogeneity can be constructed from this by linear superposition: Multiplying both sides with $a(t')$ and integrating over $\mathrm{d}t'$ gives

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\right)\underbrace{\int \mathrm{d}t'\, G(t-t')a(t')}_{=x(t)} = \int \mathrm{d}t' \delta_D(t-t')a(t') = a(t) \tag{X.562}$$

such that the solution for the amplitude as a function of time has to be given by

$$x(t) = \int \mathrm{d}t'\, G(t-t')a(t') \tag{X.563}$$

i.e. as a convolution relation over the excitation $a(t)$. The interpretation of the response $G(t-t')$ as defined by eqn. (X.561) would now be the solution to the dynamical system to an infinitely sharp excitation. Actually, this is sensible, as it would in fact contain all possible Fourier-modes, even at equal amplitude. But is it possible to construct the Green-function explicitly from the differential operator? After all, the inhomogeneity $a(t)$ is taken care of by the integration eqn. (X.563) and the Green-function itself is defined formally by eqn. (X.561): In fact, in Fourier-space this relation reads:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\right)G(t-t') = \left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}}{\mathrm{d}t} + \omega_0^2\right)\int \frac{\mathrm{d}\omega}{2\pi}\, G(\omega)\exp(\mathrm{i}\omega t) =$$
$$\int \frac{\mathrm{d}\omega}{2\pi}\left(-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2\right)G(\omega)\exp(\mathrm{i}\omega t) = \int \frac{\mathrm{d}\omega}{2\pi}\exp(\mathrm{i}\omega t) = \delta_D(t-t') \tag{X.564}$$

such that

$$G(\omega) = \frac{1}{-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2} \tag{X.565}$$

with the inverse transform

$$G(t-t') = \int \frac{\mathrm{d}\omega}{2\pi}\, G(\omega)\exp(\mathrm{i}\omega(t-t')) = \int \frac{\mathrm{d}\omega}{2\pi}\,\frac{1}{-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2}\exp(\mathrm{i}\omega(t-t')) \tag{X.566}$$

which can be shown to be a Lorentzian ✈ spectral line profile.

To complete the analogy to electrodynamics it's instructive to think of the inhomogeneity ρ in electrostatic Poisson-equation $\Delta\Phi = -4\pi\rho$ as the external driving that perturbs the solution to the ✈ Laplace equation $\Delta\Phi = 0$. The resulting Green-function $G(\omega)$ is complex-valued; its real and imaginary parts are depicted in Fig. 35, along with its modulus and phase.

A more complete view is presented in Fig. 36, where the Green-function is shown with the phase in color and the modulus in hue.

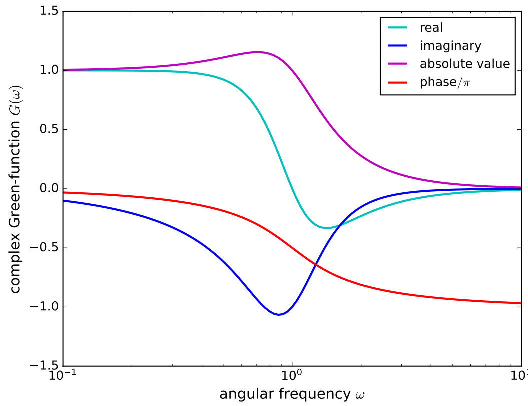

Figure 35: Complex-valued Green-function G(ω) *for the damped harmonic oscillator, for* $\omega_0 = \gamma = 1$*, specifically the real and imaginary parts as well as the modulus and the phase angle.*

An external, sinusoidal driving would correspond to a choice of a value for ω on the real axis, and a value close to the two singularities would result in resonant driving. The singularities are situated at

$$\omega^2 - i\gamma\omega - \omega_0^2 = 0 \quad \rightarrow \quad \omega_\pm = \frac{i\gamma \pm \sqrt{4\omega_0^2 - \gamma^2}}{2}, \tag{X.567}$$

i.e. at $\sqrt{3}/2 + i/2$ for the numerical example with $\omega_0 = \gamma = 1$.

Fig. 37 shows spectra for a range of musical instruments. All spectra show the harmonic series of integer multiples of the base note. Their relative amplitudes determine the sound of the respective instruments.

Fig. 38 illustrates, how incredibly well-fitting the Lorentzian line shape for spectra lines actually is. From this observation, one might conclude that a damped harmonic oscillator with an external driving is a good mechanical model for the sound generation in a musical instrument, and motivates sound engineering in a synthesiser.

X.6 *Spherical harmonics*

It is well possible to construct complete orthonormal systems of functions on other manifolds, for instance on the surface of a sphere. As in the case of plane waves for Euclidean space with Cartesian coordinate, which solve the Helmholtz differential equation, one can look for the set of solutions to the wave equation

$$\Delta Y_{\ell m}(\theta,\varphi) = -\ell(\ell+1)Y_{\ell m}(\theta,\varphi) \quad \rightarrow \quad [\Delta + \ell(\ell+1)]\, Y_{\ell m}(\theta,\varphi) = 0 \tag{X.568}$$

where the Laplace-operator is a differentiation with respect to the angular coordinate θ and φ. Comparing to the Cartesian Helmholtz-PDE $\left[\Delta + k^2\right]\exp(\pm k_i r^i) = 0$ one identifies the term $\ell(\ell+1)$ with k^2, implying that π/ℓ should be a wave length (in terms of radians) just like $2\pi/k$ would be a physical wave length λ.

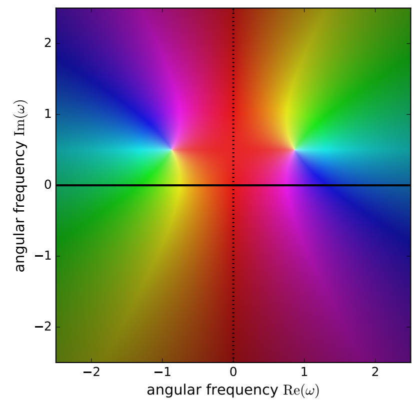

Figure 36: Complex-valued Green-function G(ω) *over the complex plane* ω = Re(ω) + i Im(ω)*, with phase indicated by colour and absolute value by hue, again for* $\omega_0 = \gamma = 1$*.*

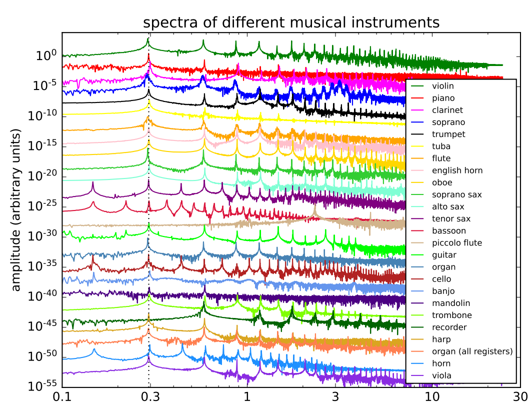

Figure 37: Spectra of different musical instruments, showing higher-order harmonics.

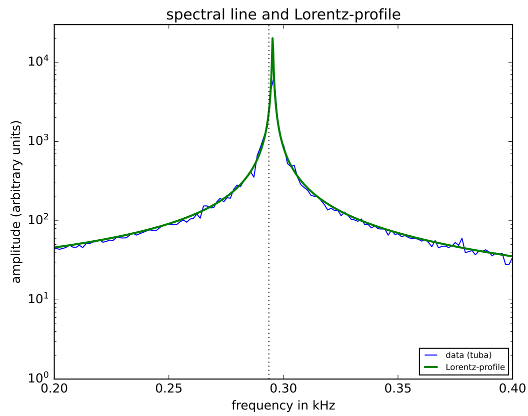

Figure 38: Spectral line of a tone with a best-fitting Lorentz-profile.

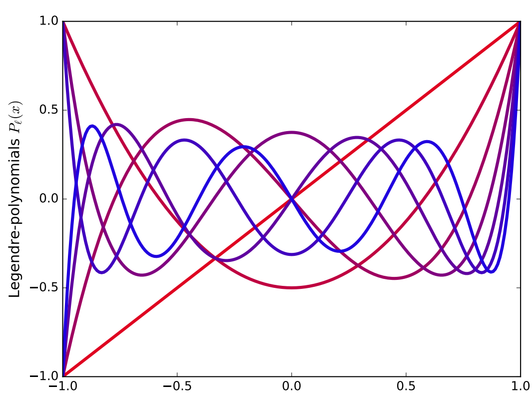

Figure 39: Legendre polynomials $P_\ell(x)$ for $\ell = 1 \dots 8$, with even parity for even ℓ, and odd parity for odd ℓ.

The Laplace-operator Δ in angular coordinates applied onto a scalar function $\psi(\theta, \varphi)$ reads explicitly

$$\Delta\psi = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} \tag{X.569}$$

As there are no mixed derivatives one should try a separation ansatz

$$\psi(\theta, \varphi) = T(\theta)P(\varphi) \tag{X.570}$$

so that the Helmholtz-PDE becomes

$$\Delta\psi = \frac{P(\varphi)}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T(\theta)}{\partial\theta}\right) + \frac{T(\theta)}{\sin^2\theta}\frac{\partial^2 P(\varphi)}{\partial\varphi^2} = -\ell(\ell+1)T(\theta)P(\varphi) \tag{X.571}$$

such that division by $T(\theta)P(\varphi)$ separates the terms as dependent on θ or φ

$$\frac{\sin\theta}{T}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right) + \ell(\ell+1)\sin^2\theta = -\frac{1}{P}\frac{\partial^2 P}{\partial\varphi^2} \tag{X.572}$$

to the left and right side of the equation: They must therefore both be equal to a separation constant m^2. Then, the right side gives

$$\frac{1}{P}\frac{\partial^2 P}{\partial\varphi^2} = -m^2 \quad \rightarrow \quad \left(\frac{\partial^2}{\partial\varphi^2} + m^2\right)P(\varphi) = 0 \tag{X.573}$$

which is again a Helmholtz-differential equation, this time in φ only. It has wave-type solutions

$$P(\varphi) \propto \exp(\pm i m\varphi) \tag{X.574}$$

with m playing the role of a wave number, but it has to be integer because otherwise the continuity of the solution could not be ensured when rotating by 2π:

$$P(\varphi+2\pi) = P(\varphi) \quad \text{implies} \quad \exp(\pm i m(\varphi+2\pi)) = \underbrace{\exp(\pm 2\pi i m)}_{=1}\exp(\pm i m\varphi) = \exp(\pm i m\varphi) \tag{X.575}$$

if m is integer. With this knowledge we return to the θ-equation, which becomes the associated Legendre-differential equation

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{m^2}{\sin^2\theta} + \ell(\ell+1)\right]T(\theta) = 0 \tag{X.576}$$

after resorting the terms, where the particular case $m = 0$ leads to the actual Legendre-differential equation,

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right) + \ell(\ell+1)T(\theta) = 0 \tag{X.577}$$

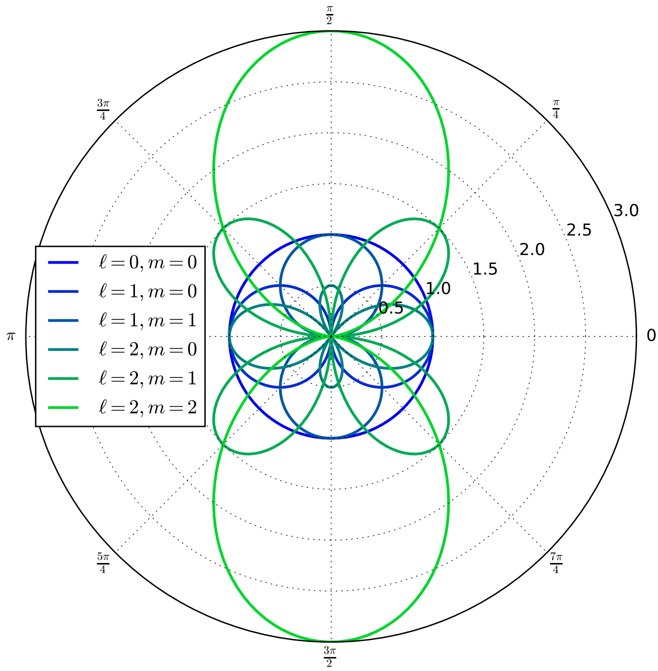

Figure 40: Associated Legendre polynomials $P_{\ell m}(\cos\theta)$ *in a polar representation.*

Transitioning to the new variable $x = \cos\theta$ with $\sin\theta = \sqrt{1-x^2}$ then yields

$$(1-x^2)\frac{d^2T}{dx^2} - 2x\frac{dT}{dx} + \ell(\ell+1)T(x) = 0 \tag{X.578}$$

whose solution are the Legendre-polynomials $P_\ell(x)$. They can be shown to obey an orthogonality relation

$$\int_{-x}^{+1} dx\, P_\ell(x)P_{\ell'}(x) = \frac{2}{2\ell+1}\delta_{\ell\ell'} \tag{X.579}$$

in the same way as the plane waves $\exp(\pm i m\varphi)$ for the azimuthal coordinate, confirming that the Helmholtz differential equation in fact defines a system of orthonormal waves on the surface of the sphere.

In the same way there is an orthogonality relation for the solutions to the associated Legendre differential equation

$$\int_{-1}^{+1} \mathrm{d}x \, \mathrm{P}_{\ell m}(x)\mathrm{P}_{\ell' m'}(x) = \frac{2}{2\ell+1}\frac{(\ell+|m|)!}{(\ell-|m|)!}\delta_{\ell\ell'}\delta_{mm'} \tag{X.580}$$

such that the definition of the spherical harmonics including the prefactors

$$\mathrm{Y}_{\ell m}(\theta,\varphi) = \sqrt{\frac{4\pi}{2\ell+1}}\sqrt{\frac{(\ell-|m|)!}{(\ell+|m|)!}}\mathrm{P}_{\ell m}(\cos\theta)\exp(+\mathrm{i}m\varphi) \tag{X.581}$$

gives the fundamental orthogonality

$$\int_{4\pi} \mathrm{d}\Omega \, \mathrm{Y}_{\ell m}(\theta,\varphi)\mathrm{Y}^*_{\ell' m'}(\theta,\varphi) = \delta_{\ell,\ell'}\delta_{mm'} \tag{X.582}$$

and completeness relations

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} \mathrm{Y}_{\ell m}(\theta,\varphi)\mathrm{Y}^*_{\ell m}(\theta',\varphi') = \delta_\mathrm{D}(\theta-\theta')\delta_\mathrm{D}(\varphi-\varphi') \tag{X.583}$$

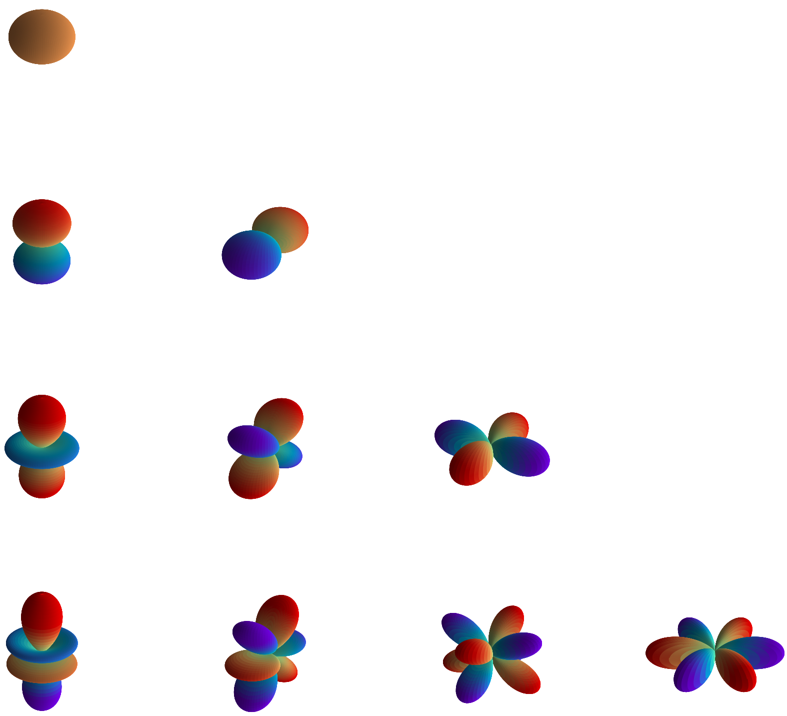

Figure 41: Spherical harmonics $Y_{\ell m}(\theta, \varphi)$ *for* $\ell = 0, 1, 2, 3$ *(top to bottom) and* $0 \leq m \leq \ell$ *(corresponding rows).*